

Quantum state discrimination: a geometric approach

Damian Markham*

*Université Paris 7, 175 Rue du Chevaleret, 75013 Paris, France and
Department of Physics, Graduate School of Science, University of Tokyo, Tokyo 113-0033, Japan*

Jarosław Adam Miszczak[†] and Zbigniew Puchała[‡]

*Institute of Theoretical and Applied Informatics,
Polish Academy of Sciences, Bałtycka 5, 44-100 Gliwice, Poland*

Karol Życzkowski[§]

*Instytut Fizyki im. Smoluchowskiego, Uniwersytet Jagielloński, ul. Reymonta 4, 30-059 Kraków, Poland and
Centrum Fizyki Teoretycznej, Polska Akademia Nauk, Al. Lotników 32/44, 02-668 Warszawa, Poland*

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We analyse the problem of finding sets of quantum states that can be deterministically discriminated. From a geometric point of view this problem is equivalent to that of embedding a simplex of points whose distances are maximal with respect to the Bures distance (or trace distance). We derive upper and lower bounds for the trace distance and for the fidelity between two quantum states, which imply bounds for the Bures distance between the unitary orbits of both states. We thus show that when analysing minimal and maximal distances between states of fixed spectra it is sufficient to consider diagonal states only. Hence considering optimal discrimination, given freedom up to unitary orbits, it is sufficient to consider diagonal states. This is illustrated geometrically in terms of Weyl chambers.

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I. INTRODUCTION

The geometry of state space depends on the distance measure chosen. In state discrimination, given a set of possible states, our task is to find out as ‘best’ as possible which of the states we have in our possession [1, 2, 3]. Finding an optimal procedure of unambiguous discrimination is particularly interesting if the states analyzed are mixed [4, 5, 6, 7, 8]. The usual approach to the quantum discrimination problem is to begin by considering the classical case and then extending to the quantum case. Different concepts of ‘best’ induce different measures of distinguishability in the space of classical probability distributions. In the quantum case, on top of the statistical uncertainty of states, even pure states cannot be always be perfectly discriminated (if the states are not orthogonal), meaning that one has to be careful in extending these to the quantum setting. To do this we bring it back to the classical setting of probability distributions by maximising over all possible discrimination measurements. In this way the problem of discriminating quantum states has led to several distance measures associated with the ability to discriminate well (see e.g. [9, 10, 11]). In this work we would like to consider the geometry induced by these measures, and how the problem of state discrimination can be expressed geometrically.

More precisely, let \mathcal{M}_N denote the set of mixed quantum states acting on an N dimensional Hilbert space \mathcal{H}_N . It is a convex, compact set of dimensionality $N^2 - 1$. Its geometric structure depends on the metric used. The following distances are often used [10, 11]

$$D_{\text{HS}}(\rho_1, \rho_2) := [\text{Tr}(\rho_1 - \rho_2)^2]^{1/2}, \quad (1.1)$$

$$D_{\text{tr}}(\rho_1, \rho_2) := \frac{1}{2} \text{Tr}|\rho_1 - \rho_2|, \quad (1.2)$$

$$D_{\text{B}}(\rho_1, \rho_2) := (2[1 - \text{Tr}|\sqrt{\rho_1}\sqrt{\rho_2}|])^{1/2}, \quad (1.3)$$

*Electronic address: markham@phys.s.u-tokyo.ac.jp

[†]Electronic address: miszczak@iitis.gliwice.pl

[‡]Electronic address: z.puchala@iitis.gliwice.pl

[§]Electronic address: karol@cft.edu.pl

denoting the Hilbert-Schmidt (HS) distance, the trace distance and the Bures distance respectively. The latter quantity is a function of *fidelity* [12],

$$F(\rho_1, \rho_2) := [\text{Tr}|\sqrt{\rho_1}\sqrt{\rho_2}|]^2, \quad (1.4)$$

and the root fidelity \sqrt{F} , (which in some papers is also called ‘fidelity’). The Bures and the trace distance are *monotone*, and do not grow under the action of an arbitrary quantum operation (completely positive, trace preserving map), while the Hilbert-Schmidt (HS) distance is not monotone. These measures can induce different geometries. For instance, the set \mathcal{M}_2 of mixed states of a qubit, is equivalent to the standard Bloch-ball (the Bloch-sphere and its interior) for the trace or HS metric, and to Uhlmann hemisphere, $\frac{1}{2}S^3$, for the Bures distance [13]. For higher N the geometries induced by the HS and the trace distance also differ.

In the following we consider systems of dimension N greater or equal to two. We begin our discussion of state discrimination by introducing the diameter of a set of quantum states. The diameter of the set \mathcal{M}_N is independent of N , but it does depend on the metric used: the *diameter* is the maximal distance between any two states, and it reads

$$D_{\text{HS}}^{\text{max}} = \sqrt{2}, \quad D_{\text{tr}}^{\text{max}} = 1, \quad D_{\text{B}}^{\text{max}} = \sqrt{2}, \quad (1.5)$$

for HS, trace and Bures distances, respectively. Any two states separated by D^{max} are supported on orthogonal subspaces. The reverse implication holds for Bures and trace distances,

$$\text{supp}(\rho_1) \perp \text{supp}(\rho_2) \Leftrightarrow D_{\text{tr}}(\rho_1, \rho_2) = 1 \Leftrightarrow D_{\text{B}}(\rho_1, \rho_2) = \sqrt{2}, \quad (1.6)$$

but is not true for the Hilbert-Schmidt distance for $N > 2$. For instance, the HS distance between two diagonal density matrices $\rho_1 = \text{diag}(1, 0, 0)$ and $\rho_2 = \text{diag}(0, 1/2, 1/2)$ is equal to $\sqrt{3/2} < D_{\text{HS}}^{\text{max}}$, although they are supported on orthogonal subspaces. To witness an even more dramatic example consider the Hilbert space of even dimension N and two diagonal states, $\rho_1 = \text{diag}(N/2, \dots, N/2, 0, \dots, 0)$ and $\rho_2 = \text{diag}(0, \dots, 0, N/2, \dots, N/2)$. Although they live in orthogonal subspaces, so their Bures and trace distances are maximal, their HS distance reads $2/\sqrt{N}$ and tends to zero in the limit of large N . This indicates that when analysing problems of distinguishability, one cannot therefore rely on the standard Euclidean geometry induced by the Hilbert-Schmidt distance, but rather better use Bures or trace distances.

The trace distance and the Bures distance are, in several respects, good measures for quantifying the ability to discriminate states. In [14] Englert introduced the notion of *distinguishability* between two quantum states and showed that it is equal to the trace distance between them. Hence two states can be deterministically discriminated if they can be perfectly distinguished, so their distinguishability is equal to unity. Fuchs and van de Graaf found a bound between the Bures distance and the trace distance based on the following inequality [10]

$$1 - \sqrt{F(\rho_1, \rho_2)} \leq D_{\text{tr}}(\rho_1, \rho_2) \leq \sqrt{1 - F(\rho_1, \rho_2)}. \quad (1.7)$$

This implies that if the fidelity between both states is equal to zero (so the states are distinguishable and their Bures distance is maximal) their trace distance is equal to unity, and is hence maximal. In fact, the trace distance is a simple function of the probability to successfully discriminate two states in a single shot measurement (optimised over all allowed quantum measurements) [10]. Similarly, the Bures distance can be seen as the optimised Kullback-Leibler distance between output statistics over all quantum measurements (again, an optimized cost function for discrimination) [9].

In the special case where both density matrices are diagonal, and read p and q , the operators commute. Such a case is often called classical since the distances between quantum states reduce then exactly to their classical analogues: The trace distance $D_{\text{tr}}(p, q)$ is the equal to the L_1 distance (with a normalisation constant $1/2$) between both probability vectors; The Bures distance reads $D_{\text{B}}(p, q) = [2(1 - B(p, q))]^{1/2}$, where

$$B(p, q) := \sum_{i=1}^N \sqrt{p_i q_i} \quad (1.8)$$

denotes the *Bhattacharyya* coefficient [15], [11]. This quantity is equal to the root fidelity between any two diagonal states, $B(p, q) = \sqrt{F(p, q)}$, so its square B^2 , is sometimes called *classical fidelity* between to probability distributions.

In section IV we prove general bounds for the fidelity between arbitrary two quantum states ρ_1 and ρ_2 ,

$$B^2(p^\uparrow, q^\downarrow) \leq F(\rho_1, \rho_2) \leq B^2(p^\uparrow, q^\uparrow), \quad (1.9)$$

where the vectors p and q represent the spectra of ρ_1 and ρ_2 , while the arrows up (down) indicate that the eigenvalues are put in the nondecreasing (nonincreasing) order. These results imply equivalent bounds for the Bures distance

$$\sqrt{2 - 2\sqrt{p^\uparrow \cdot q^\uparrow}} \leq D_B(\rho_1, \rho_2) \leq \sqrt{2 - 2\sqrt{p^\uparrow \cdot q^\downarrow}}. \quad (1.10)$$

Analogous bounds for the trace distance proved in the same section read

$$D_{\text{tr}}(p^\uparrow, q^\uparrow) \leq D_{\text{tr}}(\rho_1, \rho_2) \leq D_{\text{tr}}(p^\uparrow, q^\downarrow), \quad (1.11)$$

where the symbols p^\uparrow and q^\downarrow denote here diagonal density matrices with all eigenvalues in the increasing (decreasing) order.

In this paper we set out to give a geometric interpretation to the problem of state discrimination in terms of the geometries induced by the trace and Bures distance. We begin in section II by giving a set of conditions on states such that they may be perfectly discriminated. In section III we present some geometrical consequences of these conditions and phrase the problem of state discrimination in terms of the embedding of simplices with respect to different distance functions. In section IV we investigate the distance between states under unitary orbits and its geometric interpretation, and prove the above bounds. We finish in section V with conclusions.

II. PERFECT DISCRIMINATION OF STATES

We begin by looking at some conditions on the set of states that can be perfectly discriminated. Our condition will follow from simple analysis of the measurements (in terms of the associated positive operator valued measure (POVM)), and give general conditions which, in the next section, will be used to give some geometrical consequences of the problem.

Theorem 1 *Two states ρ_1 and ρ_2 can be deterministically discriminated iff their supports do not overlap.*

Proof. Any perfect state discrimination strategy for two states ρ_1, ρ_2 can be written as a three element POVM $\{A_1, A_2, A_?\}$, where the outcomes correspond to concluding it is the state ρ_1, ρ_2 and allowing for inconclusive outcome respectively.

Note that although in general we can have far more possible outcomes than three, this formalism does include all possible discrimination strategies - this is because we can always group the outcomes corresponding to state ρ_1 to give A_1 , and those to state ρ_2 to give A_2 , and the remaining elements we group to give $A_?$. The probability of success of the strategy can always be written in terms of such POVMs, thus we can restrict ourselves to only these three element POVMs for perfect discrimination.

The conditions on the POVM for deterministic state discrimination are

$$\text{Tr}(A_1 \rho_1) = 1 \quad (2.1)$$

$$\text{Tr}(A_2 \rho_2) = 1 \quad (2.2)$$

$$A_1 + A_2 + A_? = \mathbf{I} \quad (2.3)$$

$$\mathbf{I} \geq A_i \geq 0 \quad (2.4)$$

(this is the same logic as in [16], only without the separability condition). The first two are necessary for perfect state discrimination, and the last two are just the conditions for $\{A_i\}$ to be a POVM.

Conditions (2.1) and (2.2) imply that the elements A_1 and A_2 include projections onto the support of ρ_1 and ρ_2 respectively. To see this, rewrite (2.1) in the eigenbasis of $\rho_1 = \sum_i \lambda_i |i\rangle\langle i|$ (we extend this basis to the full space for writing A_1 in (2.6))

$$\begin{aligned} \text{Tr}(A_1 \rho_1) &= \sum_i \lambda_i \langle i|A_1|i\rangle \\ &= \sum_i \lambda_i q_i = 1, \end{aligned} \quad (2.5)$$

where $q_i := \langle i|A_1|i\rangle$ is a probability, hence $\sum_i \lambda_i q_i \leq 1$ and equality is obtained only when $q_i = 1$ for all i such that $\lambda_i \neq 0$. If we also demand conditions (2.3), (2.4) the most general A_k can be written

$$A_k = P_k + \sum_{i,j \notin \text{Supp}(\rho_1), \text{Supp}(\rho_2)} \alpha_{i,j} |i\rangle\langle j| \quad (2.6)$$

where $P_k = \sum_{i \in \text{Supp}(\rho_k)} |i\rangle\langle i|$ is the projector onto the support of state ρ_k . The support of a state ρ , with eigen-decomposition $\rho = \sum_j \alpha_j |j\rangle\langle j|$ is given by $P = \sum_j |j\rangle\langle j|$. From here, condition (2.3) clearly says

$$\begin{aligned} P_1 + P_2 &\leq \mathbf{I} \\ \Rightarrow \text{Tr}(P_1 P_2) &= 0 \\ \Rightarrow \text{Tr}(\rho_1 \rho_2) &= 0 \\ \Rightarrow \text{Tr}|\rho_1 - \rho_2|/2 &= 1. \end{aligned} \tag{2.7}$$

Hence the supports have zero overlap. □

The theorem is easily extended to sets of states $\{\rho_i\}_{i=1}^M$.

Theorem 2 *The states $\{\rho_i\}_{i=1}^M$ can be deterministically discriminated iff their supports do not overlap.*

This directly leads to

Proposition 1 *Consider K states acting on the N dimensional Hilbert space, which can be discriminated deterministically. Then*

$$\sum_{i=1}^K \text{rank}(\rho_i) \leq N. \tag{2.8}$$

This proposition is clear from the theorem, but also can be derived from the result in [16]. This is done by taking the zero entanglement case of the main result presented there. Specifically, the left hand inequality in equation (8) for zero entanglement, along with equation (1) in [16] give exactly (2.8).

III. SOME GEOMETRICAL CONSEQUENCES

We now look at what the above results have to say in terms of the geometric interpretation of the problem of state discrimination. Due to property (1.6) the above theorem can also be formulated as the condition that the trace (or Bures) distance between states are maximal. This fact has an immediate geometric implication. Let us start to work with the trace distance and denote by $\Delta_k \in \mathbb{R}^k$ a maximal regular k -simplex defined by $k+1$ points with mutual trace distance between points equal to $D_{tr}^{\max} = 1$.

Proposition 2 *Let R be an arbitrary convex subset of \mathcal{M}_N . Assume that there exists a simplex $\Delta_k \subset R$ and assume that R does not contain Δ_{k+1} . Then the maximal number of states of R which can be discriminated deterministically is equal to $k+1$.*

An analogous of the Proposition 2 may be formulated for the geometry induced by the Bures distance.

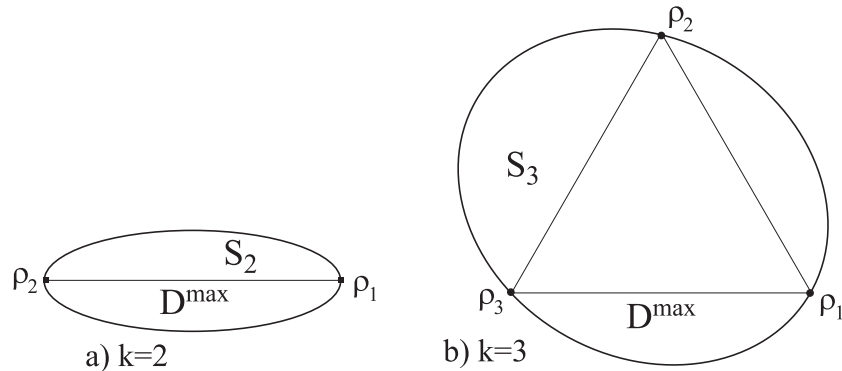


FIG. 1: Set of positive operators ρ_1, \dots, ρ_k with a) $k=2$ and b) $k=3$ distinguishable states which form a maximal simplex of size k with side length D^{\max} , with respect to the Bures (or the trace) metric.

Thus the problem of finding the maximal number of distinguishable states on a certain set is equivalent to the problem of embedding inside it a regular simplex of maximal dimensionality with the diameter given by D^{\max} (see Fig. 1).

At this point it is worth mentioning a different quantum problem of finding ‘symmetric, informationally complete positive operational valued measures’ (SIC POVM) [17]. This has a similar geometric interpretation of inscribing inside the set \mathcal{M}_N of mixed states an $N^2 - 1$ dimensional simplex spanned by N^2 pure states $|\phi_j\rangle$, the overlap of which is constant, $F = |\langle\phi_i|\phi_j\rangle|^2 = 1/(N+1)$ for any $i \neq j$. Therefore, in this case, the side of the simplex with respect to the Bures distance reads $D_B^{\text{SIC}} = \sqrt{2(1-\sqrt{F})} = \sqrt{2-2/\sqrt{N+1}}$, and for a finite dimension N , this is smaller than $D_B^{\max} = \sqrt{2}$.

So in the distinguishability problem we wish to embed into the set \mathcal{M}_N of mixed states a simplex of the maximal side length D_B^{\max} with dimensionality not larger than N , while in the SIC POVM problem we try to inscribe inside the same set a higher dimensional simplex of a smaller side length D_B^{SIC} .

IV. DISTANCES BETWEEN UNITARY ORBITS

In this section we shall be concerned with the distances between orbits generated from quantum states by unitaries. That is, given two states ρ_1 and ρ_2 with fixed spectra, we wish to know how “far” or how “close” we can make these states by unitary action. We will find that for the Bures and trace distance, the closest and the farthest that can be achieved is given when both states are diagonal in the same basis. This has a geometric interpretation in terms of the Weyl chambers as will be discussed.

This problem can be interesting in many areas of quantum information. Operationally the problem of finding the best unitary separation of two density matrices may be interesting if we are restricted to certain spectra or mixedness. For example in coding for noisy channels. If we know that the output of some channel will imply a certain mixedness (or even specific spectra), we naturally want to choose to encode on states that are least affected by this. If we are encoding classical information, this would be those states which remain most distinguishable afterwards. A simple example of such a channel would be one which probabilistically adds white noise. Freedom of the input state would correspond to unitary freedom of the outputs states which we wish to optimise over, hence considering the optimum over unitary orbits of the output mixed states is equal to finding the optimum encoding. We will see that in such cases, when only the spectra are restricted, the worst and best cases are given by taking them diagonal in the same basis.

Consider first two classical, N -point, normalised probability distributions, $p = (p_1, \dots, p_N)$ and $q = (q_1, \dots, q_N)$ such that $p_i, q_i \geq 0$ and $\sum_i p_i = \sum_i q_i = 1$. As earlier, let p_i^\downarrow denote the vector ordered decreasingly, $p_i^\downarrow \geq p_{i+1}^\downarrow$, while let p_i^\uparrow represent components of the probability vector in the increasing order: $p_i^\uparrow \leq p_{i+1}^\uparrow$.

Any quantum state ρ_1 generates an orbit of unitarily equivalent states, $U\rho_1 U^\dagger$. Two states ρ_1 and $U\rho_1 U^\dagger$ are sometimes called *geometrically uniform* and they have been recently considered in the context of unambiguous discrimination [4, 5, 8].

We are going to discuss another problem of distinguishing states from two orbits. Consider two diagonal quantum states, $\rho_1 = \text{diag}(p)$ and $\rho_2 = \text{diag}(q)$, from which we two orbits of unitarily equivalent states. We shall analyze the minimal and maximal distance D_x between the orbits,

$$M(\rho_1, \rho_2) := \max_{U, V} D_x(U\rho_1 U^\dagger, V\rho_2 V^\dagger) = \max_W D_x(\rho_1, W\rho_2 W^\dagger), \quad (4.1)$$

$$m(\rho_1, \rho_2) := \min_{U, V} D_x(U\rho_1 U^\dagger, V\rho_2 V^\dagger) = \min_W D_x(\rho_1, W\rho_2 W^\dagger), \quad (4.2)$$

since performing maximization over two unitary matrices U and V is equivalent to find a single unitary matrix $W = U^\dagger V$. Here D_x stands for one of the monotone distances D_B or D_{tr} . A similar statement for the non monotone Hilbert-Schmidt distance (1.1) was already proved in [18].

We conjecture that extrema for these distances are obtained for diagonal matrices. Then the extremization has to be performed only over the group P of permutation matrices, which change the order of the spectra,

$$M(\rho_1, \rho_2) = \max_P D_x(p, q) = D_x(p^\downarrow, q^\uparrow) = D_x(p^\uparrow, q^\downarrow), \quad (4.3)$$

$$m(\rho_1, \rho_2) = \min_P D_x(p, q) = D_x(p^\downarrow, q^\downarrow) = D_x(p^\uparrow, q^\uparrow). \quad (4.4)$$

The minimum is then achieved for the same order of components in both vectors, while the maximum occurs for opposite ordering so using the above formula one can evaluated analytically the extremal distances for both distances in consideration.

Let us first show that this conjecture holds for the Bures distance.

Theorem 3 *The maximum and minimum Bures distance between the unitary orbits of two states are given by diagonal states with*

$$M(\rho_1, \rho_2) = \max_p D_B(p, q) = D_B(p^\dagger, q^\dagger) = D_B(p^\dagger, q^\dagger), \quad (4.5)$$

and

$$m(\rho_1, \rho_2) = \min_p D_B(p, q) = D_B(p^\dagger, q^\dagger) = D_B(p^\dagger, q^\dagger). \quad (4.6)$$

Proof. a) We start by providing an upper bound for the Bures distance (1.3):
Let us start with the inequality

$$\sqrt{p^\dagger} \cdot \sqrt{q^\dagger} \geq \text{Tr} \sqrt{\rho_1} \sqrt{\rho_2} \geq \sqrt{p^\dagger} \cdot \sqrt{q^\dagger} \quad (4.7)$$

which is a particular case of (A1) from lemma 3 proved in appendix A. Since $\text{Tr} |\sqrt{\rho_1} \sqrt{\rho_2}| \geq \text{Tr} \sqrt{\rho_1} \sqrt{\rho_2}$, we immediately infer that the root fidelity is bounded from below by the Bhattacharayya coefficient between the spectra put in an opposite order,

$$\sqrt{F(\rho_1, \rho_2)} = \text{Tr} |\sqrt{\rho_1} \sqrt{\rho_2}| \geq \text{Tr} \sqrt{\rho_1} \sqrt{\rho_2} \geq \sqrt{p^\dagger} \cdot \sqrt{q^\dagger} = B(p^\dagger, q^\dagger). \quad (4.8)$$

This implies an upper bound for the Bures distance which is clearly achievable, $M(\rho_1, \rho_2) = D_B(p^\dagger, q^\dagger)$. \square

In this way we obtain a general upper bound (4.5) for the Bures distance between any two density operators with spectra p and q ,

$$D_B(\rho_1, \rho_2) \leq D_B(p^\dagger, q^\dagger) = [2(1 - \sqrt{p^\dagger} \cdot \sqrt{q^\dagger})]^{1/2}. \quad (4.9)$$

b) Next we provide a lower bound for the Bures distance (1.3):

To prove the case for minimisation our task is to show

$$\sqrt{p^\dagger} \cdot \sqrt{q^\dagger} \geq \text{Tr} |\sqrt{\rho_1} \sqrt{\rho_2}|, \quad (4.10)$$

or equivalently, to get an upper bound for the root fidelity $\sqrt{F(\rho_1, \rho_2)}$.

First we note that for any operator A we have [10, 19, 24]

$$\max_U |\text{Tr} U A| = \text{Tr} \sqrt{A A^\dagger} \equiv \text{Tr} |A| \equiv \|A\|_1, \quad (4.11)$$

where the maximum is taken over all unitaries U . We will also use the inequality of von Neumann inequality [20], which concerns absolute value of the trace of a product of two matrices and their singular values.

Lemma 1 (von Neumann inequality) *Let $\sigma_1(A), \dots, \sigma_n(A)$ and $\sigma_1(B), \dots, \sigma_n(B)$ denote singular values of the matrices A and B arranged in nonincreasing order. For any matrices A and B the following inequality holds*

$$|\text{Tr} AB| \leq \sum_{i=1}^n \sigma_i(A) \sigma_i(B). \quad (4.12)$$

For a recent exposition see [21] and [22].

Without loosing the generality we can assume that ρ_1 is diagonal, $\rho_1 = \text{diag}(p)$ and $\rho_2 = V \text{diag}(q) V^\dagger$. Then

$$\max_V \sqrt{F(\rho_1, \rho_2)} = \max_V \text{Tr} |\sqrt{\rho_1} \sqrt{\rho_2}| = \max_V \text{Tr} |\sqrt{p} V \sqrt{q} V^\dagger|. \quad (4.13)$$

Using (4.11) and the cyclic property of trace we get

$$\max_V \sqrt{F(\rho_1, \rho_2)} = \max_{V, U} |\text{Tr} U \sqrt{p} V \sqrt{q} V^\dagger| = \max_{V, U} |\text{Tr} \sqrt{p} V \sqrt{q} V^\dagger U| \quad (4.14)$$

$$= \max_{V, W} |\text{Tr} \sqrt{p} V \sqrt{q} W| \quad (4.15)$$

where $W = V^\dagger U$ is unitary. Since the vectors \sqrt{p} and \sqrt{q} contain singular values of matrices $\sqrt{p}V$ and $\sqrt{q}W$, respectively, it follows from (4.12) that

$$|\text{Tr} \sqrt{p}V \sqrt{q}W| \leq \sum_{i=1}^n \sigma_i^\uparrow(\sqrt{p}V) \sigma_i^\uparrow(\sqrt{q}W). \quad (4.16)$$

Thus we get the bound for the maximal root fidelity at the unitary orbit,

$$\max_V \sqrt{F}(\rho_1, \rho_2) \leq \sum_{i=1}^n \sigma_i^\uparrow(\sqrt{p}V) \sigma_i^\uparrow(\sqrt{q}W) \quad (4.17)$$

$$= \sqrt{p^\uparrow} \cdot \sqrt{q^\uparrow}. \quad (4.18)$$

This result implies the desired upper bound for the root fidelity,

$$\sqrt{F}(\rho_1, \rho_2) \leq \sqrt{p^\uparrow} \cdot \sqrt{q^\uparrow}, \quad (4.19)$$

which finishes the proof of the lower bound (4.6). Squaring the relations (4.8) and (4.19) we establish the inequalities (1.9) and (1.10). \square

Now we are going to formulate and prove an analogous conjecture for the trace distance.

Theorem 4 *The maximum and minimum trace distance between the unitary orbits of two states are given by diagonal states with*

$$M(\rho_1, \rho_2) = \max_p D_{\text{tr}}(p, q) = D_{\text{tr}}(p^\downarrow, q^\uparrow) = D_{\text{tr}}(p^\uparrow, q^\downarrow), \quad (4.20)$$

and

$$m(\rho_1, \rho_2) = \min_p D_{\text{tr}}(p, q) = D_{\text{tr}}(p^\downarrow, q^\downarrow) = D_{\text{tr}}(p^\uparrow, q^\uparrow). \quad (4.21)$$

Proof. The above theorem can be expressed in term of singular values as

$$\sum_{i=1}^n |\sigma_i(\rho_1) - \sigma_i(\rho_2)| \leq \sum_{i=1}^n \sigma_i(\rho_1 - \rho_2) \leq \sum_{i=1}^n |\sigma_i(\rho_1) - \sigma_{n+1-i}(\rho_2)|. \quad (4.22)$$

Here $\sigma_i(\rho_1)$ and $\sigma_i(\rho_2)$ denote decreasingly ordered singular values of both operators.

The lower bound follows from the special case ($k = n$) of the following lemma from [24].

Lemma 2 *Let $A, B \in M_n$, and suppose $A, B, A - B$ have decreasingly ordered singular values $\sigma_1(A) \geq \dots \geq \sigma_n(A), \sigma_1(B) \geq \dots \geq \sigma_n(B), \sigma_1(A - B) \geq \dots \geq \sigma_n(A - B)$. Define $s_i(A, B) \equiv |\sigma_i(A) - \sigma_i(B)|$ and let $s_{[1]}(A, B) \geq \dots \geq s_{[n]}(A, B)$ denote a decreasingly ordered rearrangement of the values $s_i(A, B)$. Then*

$$\sum_{i=1}^k s_{[i]}(A, B) \leq \sum_{i=1}^k \sigma_i(A - B) \text{ for } k = 1, 2, \dots, n. \quad (4.23)$$

The upper bound in (4.22) follows from lemma 5 in appendix B if A and B are positive semidefinite. Since any two density matrices, ρ_1 and ρ_2 , are hermitian and positive, their eigenvalues and singular values are equal. Making use of the definition (1.2) we obtain therefore required bounds for the trace distance

$$2D_{\text{tr}}(p^\downarrow, q^\downarrow) \leq \text{Tr}|\rho_1 - \rho_2| \leq 2D_{\text{tr}}(p^\downarrow, q^\uparrow) \quad (4.24)$$

equivalent to eq. (1.11). \square

We now consider what this means geometrically, and we will do this in terms of the so called Weyl chamber. A Weyl chamber is a simplex of ordered eigenvalues (see, e.g. [11]). Any unitary orbit is generated from an ordered spectrum of the density matrix, which corresponds to a point inside a Weyl chamber, i.e. the asymmetric $1/N!$ part

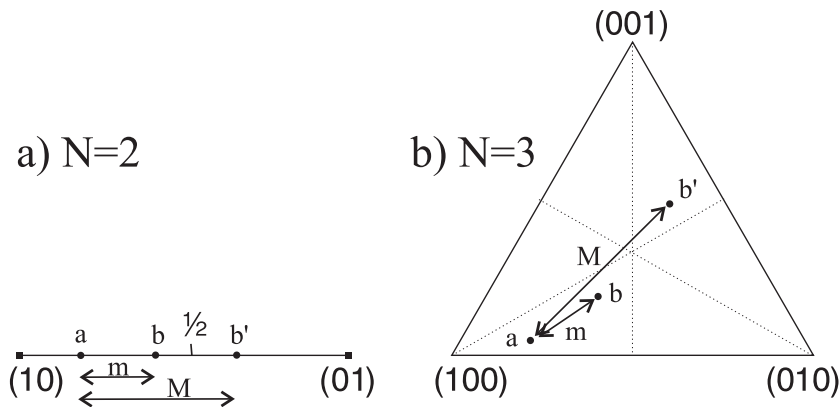


FIG. 2: The minimal distance m between the orbits of unitarily similar states stemming from two quantum states are equal to the distances between the corresponding spectra a and b belonging to the same Weyl chamber shown for a) $N = 2$ and b) $N = 3$. The maximal distance M is achieved for points a and b' belonging to the opposite Weyl chambers.

of the simplex of eigenvalues. Thus the minimal distance between a diagonal state ρ_1 and a unitary orbit stemming from ρ_2 is obtained if the orbit intersects the Weyl chamber distinguished by ρ_1 . On the other hand the maximum is achieved also for a diagonal ρ_2 with permuted spectrum, which belongs to another Weyl chamber (see Fig. 2 for $N = 2$ and $N = 3$).

Let us analyze the simplest case $N = 2$, for which the simplex of eigenvalues is equivalent to an interval $[0, 1]$, while the intervals $[0, 1/2)$ and $(1/2, 1]$ form two Weyl chambers. A unitary orbit generated by each point of a Weyl chamber has the structure of the sphere, S^2 . The above statement has an intuitive interpretation: the minimal distance between two concentric spheres is equal to the distance between two of their points belonging to the same radius of the ball. The maximal distance between these spheres equals to the distance between their points placed at the diameter of the ball on the other sides of its center. For example consider two states in the Bloch ball. The radius is given by the entropy, in this case completely defining the spectrum also. So two orbits are given by two concentric spheres of different radius. Common eigenbases corresponds to a common axis, hence the closest and furthest states both lie on the same axis, either both on the same side or opposite sides of the center respectively.

The above property shows that looking for a set of perfectly distinguishable states in a certain set S of mixed states which is invariant with respect to the unitary rotations, it is enough to analyze the subset of diagonal matrices.

Proposition 3 *Let R_Δ be an arbitrary convex subset of the $(N - 1)$ dimensional simplex of the eigenvalues. Let R denote the set of quantum states obtained from this set by any unitary rotation, $R := \{\rho \in \mathcal{M}_N : \rho = U[\text{diag}(p)]U^\dagger, \text{ and } p \in R_\Delta\}$. Let $k \leq N$ be the number such that $\Delta_{k-1} \in R_\Delta$ and there exists no $\Delta_k \in R_\Delta$. Then the maximal number of perfectly distinguishable states in R is equal to k , so it is equal to the maximal number of diagonal distinguishable states.*

As before, the symbol Δ_k represents a regular k dimensional simplex containing $k + 1$ points separated by the maximal distance D^{\max} with respect to the trace (or Bures) distance. Let us emphasise again that the geometry induced by the Bures metric differs considerably with respect to the flat Euclidean geometry induced by the HS metric. For instance, the simplex of eigenvalues for $N = 3$ forms a flat equilateral triangle (of side $\sqrt{2}$) in the HS case, while it is equivalent to the octant of a sphere S^2 for the Bures distance.

V. CONCLUSIONS

In this work we have commenced with the analysis of the geometry of the problem of quantum distinguishability. We have shown that the problem of finding the maximal number of perfectly distinguishable states in a certain set R containing quantum states is equivalent to finding the dimension of the largest simplex of a fixed side size which can be embedded inside the set R . For this purpose one cannot use Euclidean simplices defined by the HS distance, but use simplices with respect to Bures or trace distances.

Fidelity between any two quantum states is shown to be bounded by the classical fidelities between both spectra put in the same order (upper bound) or in the opposite order (lower bound). This observation implies bounds for the Bures distance between two quantum states are achieved for diagonal states. Thus looking for distinguishable states

in a rotationally invariant subset of the set of quantum states it is sufficient to restrict analysis to a smaller set of classical states, which correspond to diagonal density matrices.

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APPENDIX A: BOUND FOR THE TRACE OF A PRODUCT OF STATES

Let $\rho = \rho^\dagger$ and $\sigma = \sigma^\dagger$ denote two Hermitian operators acting on an N -dimensional Hilbert space. As throughout the paper, their spectra will be denoted by $p = \text{eig}(\rho)$ and $q = \text{eig}(\sigma)$ respectively. Let $p^\downarrow, q^\downarrow$ denote the N -element vector of eigenvalues ordered in decreasing order, while the same spectra ordered increasingly will be written as p^\uparrow and q^\uparrow . The symbol $(p^\uparrow)^s$ denotes the vector consisting of ordered elements of p^\uparrow , each component raised to power s .

Lemma 3 *Let $\rho \geq 0$ and $\sigma \geq 0$ and let s, t denote positive real numbers. Then*

$$(p^s)^\uparrow \cdot (q^t)^\downarrow \leq \text{Tr} \rho^s \sigma^t \leq (p^s)^\uparrow \cdot (q^t)^\uparrow. \quad (\text{A1})$$

Proof. Let $|\mu_i\rangle$ and $|\nu_j\rangle$ denote the eigenvectors of the states ρ and σ . We will start by finding a form of $\text{Tr} \rho^s \sigma^t$, in terms of overlaps with a doubly stochastic matrix.

$$\text{Tr} \rho^s \sigma^t = \text{Tr} \left(\sum_{i,j} p_i^s q_j^t |\mu_i\rangle \langle \mu_i | \nu_j \rangle \langle \nu_j| \right) \quad (\text{A2})$$

$$= \sum_{i,j} p_i^s q_j^t |\langle \mu_i | U | \mu_j \rangle|^2 \quad (\text{A3})$$

$$= \sum_{i,j} p_i^s q_j^t B_{i,j}, \quad (\text{A4})$$

where U is the unitary relating the two eigenbases $U|\mu_i\rangle = |\nu_i\rangle, \forall i$ and $B := \sum_{i,j} |U_{i,j}|^2 |\mu_i\rangle \langle \mu_j|$ so that $B_{ij} = |U_{ij}|^2$. Hence matrix B is by construction unistochastic [25] and thus bistochastic.

It is convenient to introduce at this place two non-normalised vectors, $|\psi\rangle := \sum p'_i |\mu_i\rangle$, and $|\phi\rangle := \sum q'_j |\mu_j\rangle$, where $p'_i = p_i^s$ and $q'_j = q_j^t$ are non-negative. Then the trace can be rewritten in the form

$$\text{Tr} \rho^s \sigma^t = \langle \psi | B | \phi \rangle. \quad (\text{A5})$$

Birkhoff's theorem [23] states that any doubly stochastic matrix can be written as a finite convex combination of permutation matrices O_i , hence we write $B = \sum_i r_i O_i$, $\sum_i r_i = 1$. Thus the extremum of a linear function of the bistochastic matrix B will be realized at one of its extremal points. There are exactly $N!$ of them, and among all possible permutations O_i the maximum is obtained if the orders of elements of both vectors are the same, while the minimum is achieved if both spectra are in opposite order,

$$\langle \psi | B | \phi \rangle = \sum_i r_i \langle \psi | O_i | \phi \rangle \geq \langle \psi | O_{\min} | \phi \rangle = (p^\uparrow)^s \cdot (q^\downarrow)^t \quad (\text{A6})$$

$$\leq \langle \psi | O_{\max} | \phi \rangle = (p^\uparrow)^s \cdot (q^\uparrow)^t. \quad (\text{A7})$$

Since all components of the vector p (and q) are non-negative raising each element to a positive exponent s (or t) will not change the order of a vector, $(p^\uparrow)^s = (p^s)^\uparrow$. Putting it all together we arrive at (A1) and complete the proof. \square

For concreteness let us write down explicitly some special cases. In the simplest case $s = t = 1$ one obtains

$$p^\uparrow \cdot q^\downarrow \leq \text{Tr} \rho \sigma \leq p^\uparrow \cdot q^\uparrow, \quad (\text{A8})$$

while setting $s = t = 1/2$ one becomes inequality (4.7) used in the proof of inequality (4.9).

An analogue of lemma 2 may be obtained in the case one of the two operators is not positive.

Lemma 4 *Consider a positive number $s > 0$ a state $\rho \geq 0$ and an Hermitian operator $\sigma = \sigma^\dagger$ not necessarily positive. Then*

$$(p^s)^\uparrow \cdot q^\downarrow \leq \text{Tr} \rho^s \sigma \leq (p^s)^\uparrow \cdot q^\uparrow. \quad (\text{A9})$$

Proof of this lemma is similar to the proof of lemma 2. In this case the vector q of eigenvalues of operator σ contains in general also negative entries, so the vector $|\phi\rangle := \sum_j q_j |\mu_j\rangle$, is given by a pseudomixture with some weights negative. Constructing unitary bases U and bistochastic matrix M one may write the analyzed trace in the form (A5) and make use of the Birkhoff theorem. Since operator ρ with spectrum p is positive, raising its components to a positive power will not change the order, $(p^\uparrow)^s = (p^s)^\uparrow$. Therefore we may perform the last step analogous to (A7) obtaining the desired result. \square

APPENDIX B: BOUND FOR THE TRACE OF A DIFFERENCE OF TWO STATES

In this appendix we prove the following lemma.

Lemma 5 *Let A and B denote hermitian matrices of size n . Let us order decreasingly their eigenvalues, $\lambda_1(A) \geq \dots \geq \lambda_n(A)$ and $\lambda_1(B) \geq \dots \geq \lambda_n(B)$. Then the following upper bound for the trace of the absolute value of the difference holds*

$$\text{Tr}|A - B| = \sum_{i=1}^n \sigma_i(A - B) \leq \sum_{i=1}^n |\lambda_i(A) - \lambda_{n+1-i}(B)|. \quad (\text{B1})$$

Proof. Let us express both operators in their eigen representation, $A = \sum_i^n p_i |\mu_i\rangle \langle \mu_i|$ and $B = \sum_i^n q_i |\nu_i\rangle \langle \nu_i|$, where for convenience we have introduced the notation $p_i = \lambda_i(A)$ and $q_i = \lambda_i(B)$. Making use of Eq. (4.11) and basic properties of the trace we get

$$\text{Tr}|A - B| = \max_U |\text{Tr} AU - \text{Tr} BU| \quad (\text{B2})$$

$$= \max_U \left| \sum_{i=1}^n p_i \langle \mu_i | U | \mu_i \rangle - q_i \langle \nu_i | U | \nu_i \rangle \right|. \quad (\text{B3})$$

Since $|\langle \mu_i | U | \mu_i \rangle| \leq 1$, $|\langle \nu_i | U | \nu_i \rangle| \leq 1$ and $\text{Tr} U = \sum_{i=1}^n \langle \mu_i | U | \mu_i \rangle = \sum_{i=1}^n \langle \nu_i | U | \nu_i \rangle$ we have

$$\text{Tr}|A - B| \leq \max \left\{ \left| \sum_{i=1}^n \xi_i p_i - \zeta_i q_i \right| : |\xi_i| \leq 1, |\zeta_i| \leq 1 \text{ for } i = 1, \dots, n, \sum_{i=1}^n \xi_i = \sum_{i=1}^n \zeta_i \right\}. \quad (\text{B4})$$

For fixed values of ξ_i and ζ_i we denote $s = \sum_{i=1}^n \xi_i p_i - \zeta_i q_i$. Let $s = c e^{i\varphi}$, we have

$$c = |s| = \left| \frac{s}{e^{i\varphi}} \right| = \left| \sum_{i=1}^n \frac{\xi_i}{e^{i\varphi}} p_i - \frac{\zeta_i}{e^{i\varphi}} q_i \right|.$$

Because $|\frac{\xi_i}{e^{i\varphi}}| \leq 1$ and $|\frac{\zeta_i}{e^{i\varphi}}| \leq 1$ we can without loss of generality assume that $s \in \mathbb{R}$. Note now that under this assumption we have

$$\max \left\{ \left| \sum_{i=1}^n \xi_i p_i - \zeta_i q_i \right| : |\xi_i| \leq 1, |\zeta_i| \leq 1 \text{ for } i = 1, \dots, n, \sum_{i=1}^n \xi_i = \sum_{i=1}^n \zeta_i \right\} \quad (\text{B5})$$

$$= \max \left\{ \left| \sum_{i=1}^n \text{Re}(\xi_i) p_i - \text{Re}(\zeta_i) q_i \right| : |\xi_i| \leq 1, |\zeta_i| \leq 1 \text{ for } i = 1, \dots, n, \sum_{i=1}^n \xi_i = \sum_{i=1}^n \zeta_i \right\} \quad (\text{B6})$$

$$= \max \left\{ \left| \sum_{i=1}^n \xi_i p_i - \zeta_i q_i \right| : -1 \leq \xi_i \leq 1, -1 \leq \zeta_i \leq 1 \text{ for } i = 1, \dots, n, \sum_{i=1}^n \xi_i = \sum_{i=1}^n \zeta_i \right\} \quad (\text{B7})$$

The term $\sum_{i=1}^n \xi_i p_i - \zeta_i q_i$ is a linear function of $2n$ variables $\xi_1, \dots, \xi_n, \zeta_1, \dots, \zeta_n$, so it reaches its extreme value at the edges of the polygon defined by

$$\left\{ -1 \leq \xi_i \leq 1, -1 \leq \zeta_i \leq 1 \text{ for } i = 1, \dots, n, \sum_{i=1}^n \xi_i = \sum_{i=1}^n \zeta_i \right\}. \quad (\text{B8})$$

Thus we can focus on the edges of the polygon

$$\left\{ \xi_i \in \{-1, 1\}, \zeta_i \in \{-1, 1\} \text{ for } i = 1, \dots, n, \sum_{i=1}^n \xi_i = \sum_{i=1}^n \zeta_i \right\}. \quad (\text{B9})$$

Note that we obtain the maximum if in the sum $\sum_{i=1}^n \xi_i p_i + (-\zeta_i) q_i$ the n maximum values of $\{p_1, \dots, p_n, q_1, \dots, q_n\}$ will be equipped with $+1$ coefficient and n minimum values with -1 . Because $p_1 \geq p_2 \geq \dots \geq p_n$ and $q_1 \geq q_2 \geq \dots \geq q_n$, we can thus write the n maximum values as

$$\max\{p_1, q_n\}, \max\{p_2, q_{n-1}\}, \dots, \max\{p_n, q_1\}, \quad (\text{B10})$$

and the n minimum values as

$$\min\{p_1, q_n\}, \min\{p_2, q_{n-1}\}, \dots, \min\{p_n, q_1\}. \quad (\text{B11})$$

So the maximum value of

$$\max \left\{ \left| \sum_{i=1}^n \xi_i p_i - \zeta_i q_i \right| : \xi_i \in \{-1, 1\}, \zeta_i \in \{-1, 1\} \text{ for } i = 1, \dots, n, \sum_{i=1}^n \xi_i = \sum_{i=1}^n \zeta_i \right\} \quad (\text{B12})$$

is equal

$$\left| \sum_{i=1}^n \max\{p_i, q_{n-i+1}\} - \min\{p_i, q_{n-i+1}\} \right| = \sum_{i=1}^n |p_i - q_{n-i+1}|. \quad (\text{B13})$$

This gives us required upper bound (B1).

□

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